

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085513.D
 Acq On : 18 Mar 2016 1:33
 Operator : UM/SJ
 Sample : H1774-10
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-15-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.099	244	246	255	rVB	67543	120147	2.68%	0.274%
2	5.487	277	280	282	rBV	3473344	3992556	89.20%	9.101%
3	6.516	367	370	372	rBV	3301545	3960822	88.49%	9.028%
4	6.653	379	382	384	rBV	3150858	4414650	98.63%	10.063%
5	6.870	399	401	404	rBV	664218	862596	19.27%	1.966%
6	7.030	413	415	418	rBV	2831955	3244964	72.50%	7.397%
7	7.442	448	451	454	rBV	2349191	2611009	58.34%	5.952%
8	7.533	456	459	461	rVB	66795	87031	1.94%	0.198%
9	8.162	511	514	516	rBV	1365237	1197028	26.74%	2.729%
10	9.236	605	608	611	rBV	3206039	4475807	100.00%	10.202%
11	9.636	641	643	644	rBV	696584	711206	15.89%	1.621%
12	9.853	659	662	663	rVB	84212	94016	2.10%	0.214%
13	9.922	665	668	669	rVV	859345	1184482	26.46%	2.700%
14	10.345	704	705	707	rVB	154968	146078	3.26%	0.333%
15	10.562	722	724	728	rBV	58884	108054	2.41%	0.246%
16	10.711	733	737	739	rVV	2436624	2895026	64.68%	6.599%
17	10.825	745	747	753	rVV	156373	249388	5.57%	0.568%
18	11.008	761	763	767	rBV3	27810	60394	1.35%	0.138%
19	11.271	782	786	787	rBV	112956	126387	2.82%	0.288%
20	11.293	787	788	791	rVB	55371	58128	1.30%	0.132%
21	11.396	795	797	801	rBV2	1134176	1612573	36.03%	3.676%
22	11.476	801	804	806	rVB	106773	132627	2.96%	0.302%
23	11.625	814	817	821	rBV2	33255	51039	1.14%	0.116%
24	11.899	839	841	842	rBV	76836	70371	1.57%	0.160%
25	11.922	842	843	846	rVV2	231770	309316	6.91%	0.705%
26	12.014	849	851	855	rVB2	91580	143795	3.21%	0.328%
27	12.196	863	867	871	rVB2	55280	105518	2.36%	0.241%
28	12.448	887	889	891	rBV	43230	47583	1.06%	0.108%
29	12.608	901	903	906	rBV	799361	725743	16.21%	1.654%
30	12.711	910	912	915	rVV	122968	150805	3.37%	0.344%
31	12.836	919	923	926	rVV	666968	687550	15.36%	1.567%
32	12.985	933	936	939	rVB	3450816	3338786	74.60%	7.611%
33	13.054	939	942	948	rBV3	31839	67381	1.51%	0.154%
34	13.168	948	952	953	rBV	42199	78608	1.76%	0.179%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085513.D
 Acq On : 18 Mar 2016 1:33
 Operator : UM/SJ
 Sample : H1774-10
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-15-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.271	959	961	962	rBV	52571	55481	1.24%	0.126%
36	13.557	980	986	988	rBV6	16439	55736	1.25%	0.127%
37	13.671	992	996	1000	rBV	70599	97245	2.17%	0.222%
38	13.785	1003	1006	1007	rBV2	52181	78392	1.75%	0.179%
39	13.877	1012	1014	1018	rVB	265633	341930	7.64%	0.779%
40	14.037	1024	1028	1029	rBV3	931993	1435397	32.07%	3.272%
41	14.185	1038	1041	1045	rBV5	35783	109442	2.45%	0.249%
42	14.379	1054	1058	1059	rBV3	22653	58839	1.31%	0.134%
43	14.414	1059	1061	1063	rVB	35963	46054	1.03%	0.105%
44	14.505	1067	1069	1071	rVV	153136	166106	3.71%	0.379%
45	14.665	1081	1083	1085	rVB	137665	147972	3.31%	0.337%
46	14.802	1093	1095	1100	rVB3	32513	55664	1.24%	0.127%
47	14.882	1100	1102	1105	rVB3	32315	59450	1.33%	0.136%
48	14.940	1105	1107	1112	rVB3	23679	58033	1.30%	0.132%
49	15.054	1114	1117	1121	rBV	235008	438584	9.80%	1.000%
50	15.157	1121	1126	1129	rBV2	123131	232694	5.20%	0.530%
51	15.351	1140	1143	1146	rVB	113695	154041	3.44%	0.351%
52	15.408	1146	1148	1151	rVB	178445	213032	4.76%	0.486%
53	15.465	1151	1153	1161	rBV	556899	974350	21.77%	2.221%
54	15.694	1171	1173	1175	rVB2	31818	44858	1.00%	0.102%
55	15.911	1190	1192	1195	rBV	41366	67959	1.52%	0.155%
56	15.968	1195	1197	1200	rVB2	30929	51107	1.14%	0.116%
57	16.871	1273	1276	1281	rVV2	74997	166280	3.72%	0.379%
58	16.974	1282	1285	1288	rVV2	28634	72094	1.61%	0.164%
59	17.054	1289	1292	1294	rVV	39616	94242	2.11%	0.215%
60	17.111	1294	1297	1304	rVB4	28568	87130	1.95%	0.199%
61	17.294	1310	1313	1319	rVB	54136	130936	2.93%	0.298%
62	17.443	1322	1326	1330	rBV4	49654	139578	3.12%	0.318%
63	18.426	1408	1412	1421	rBV3	35884	116175	2.60%	0.265%

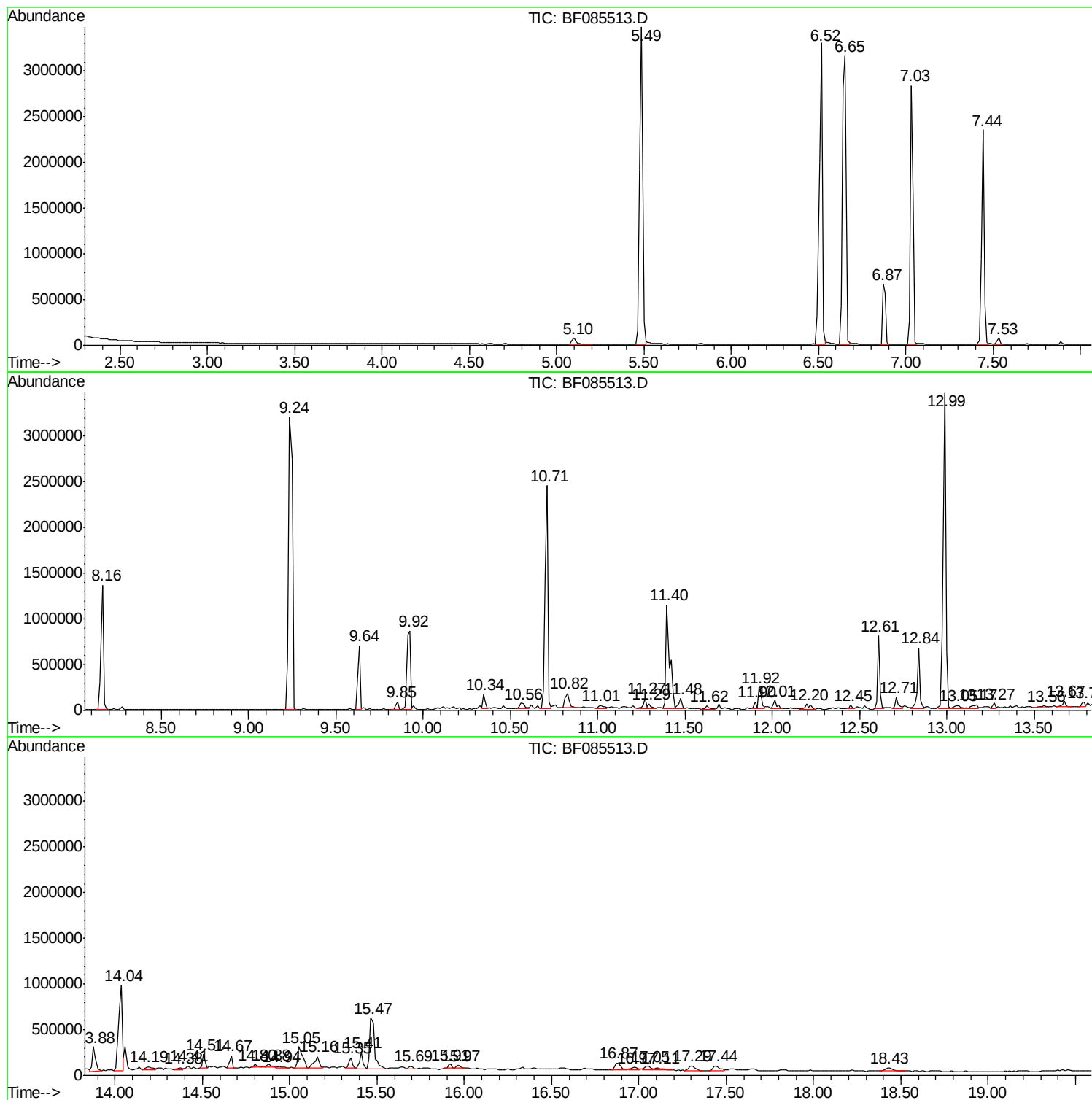
Sum of corrected areas: 43870265

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

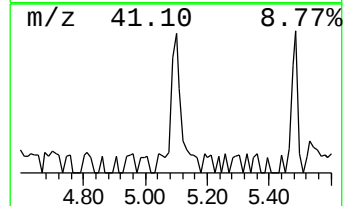
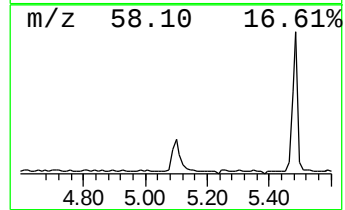
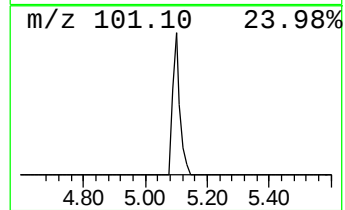
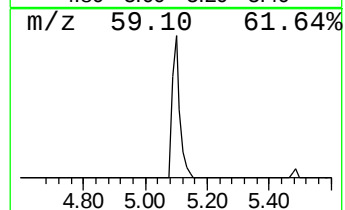
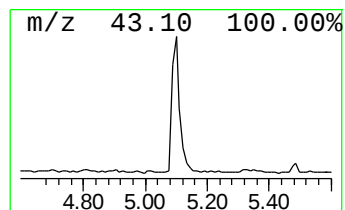
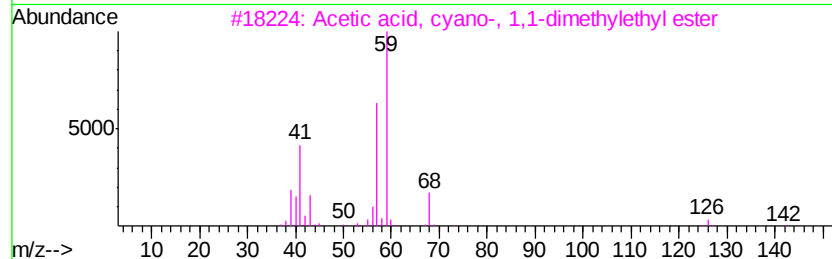
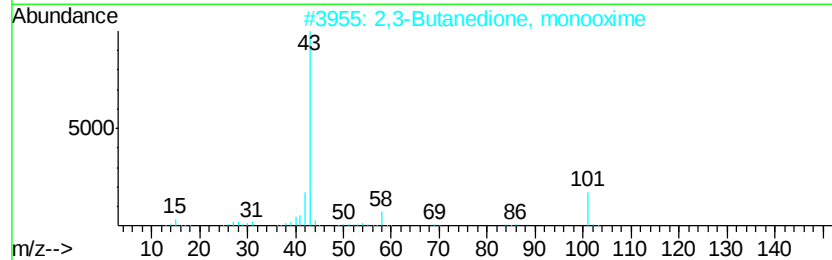
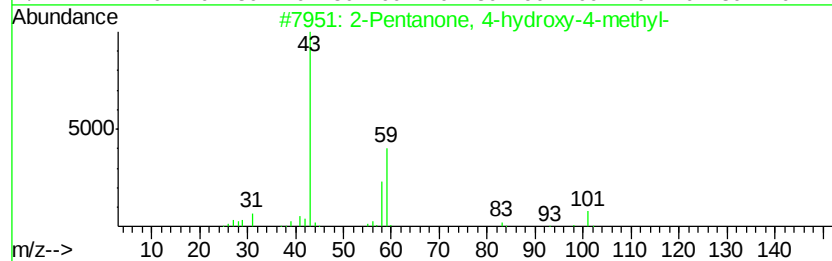
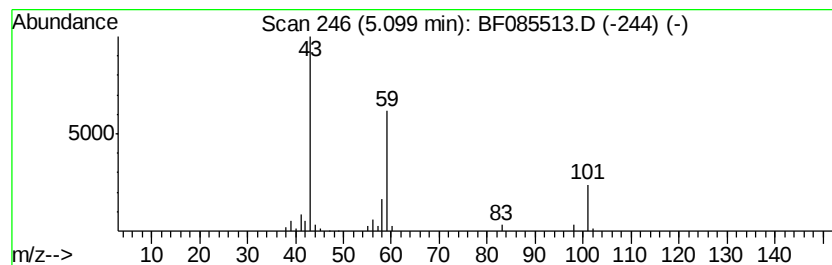
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.79 ng	120147	1,4-Dichlorobenzene-d4	6.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

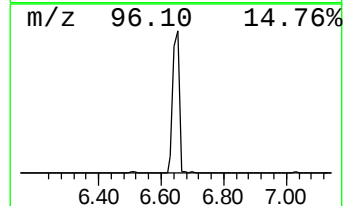
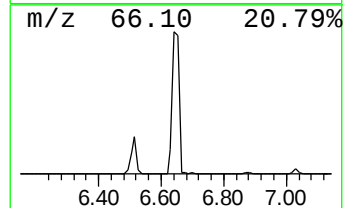
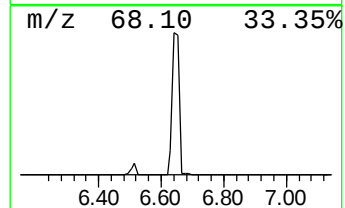
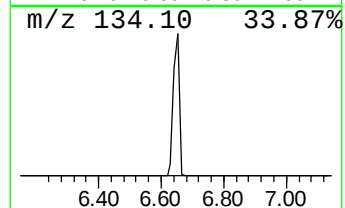
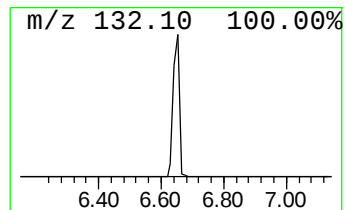
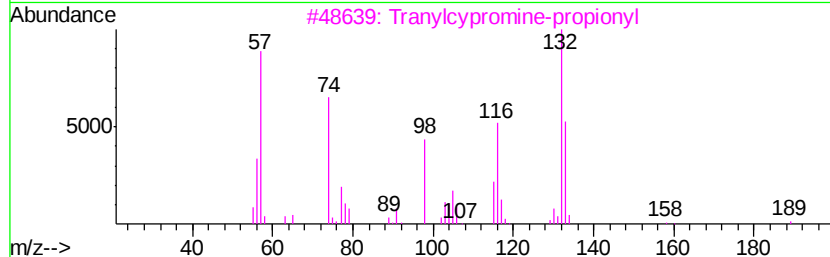
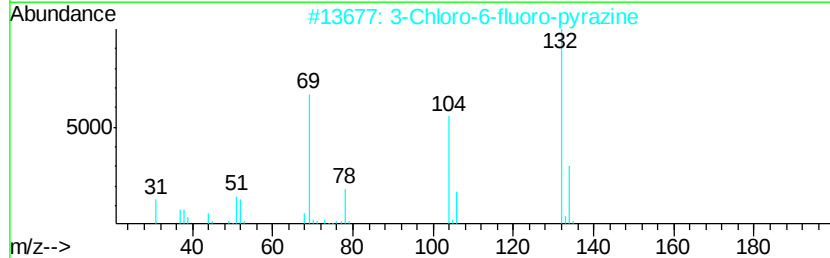
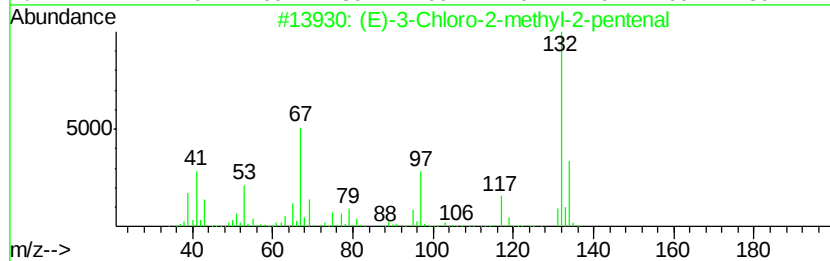
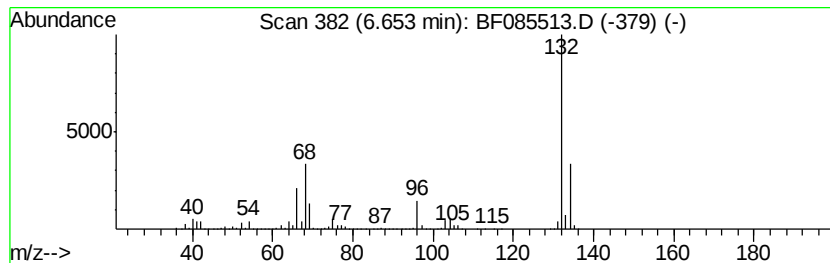
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	102.36 ng	4414650	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

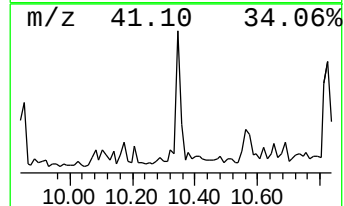
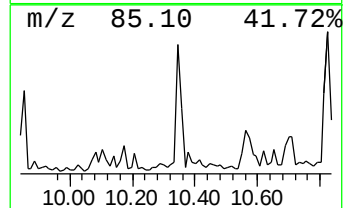
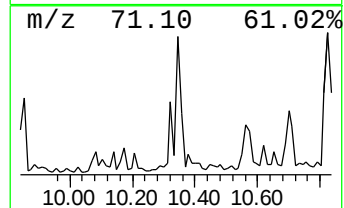
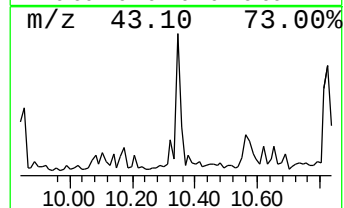
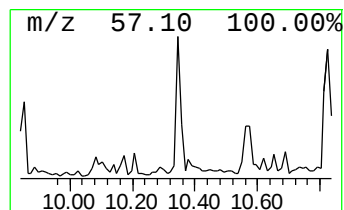
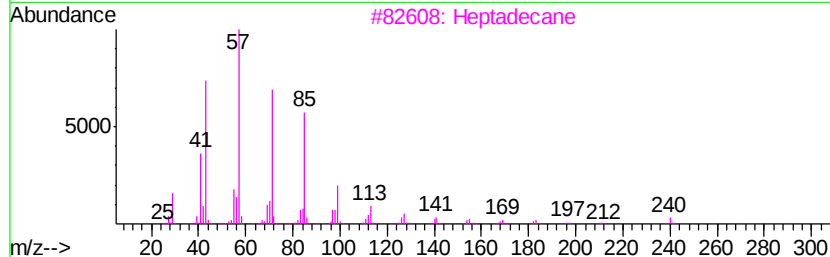
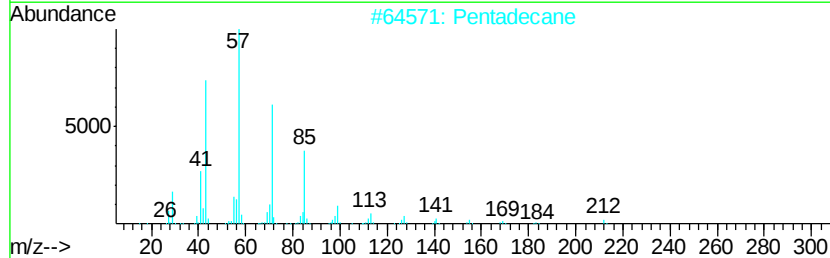
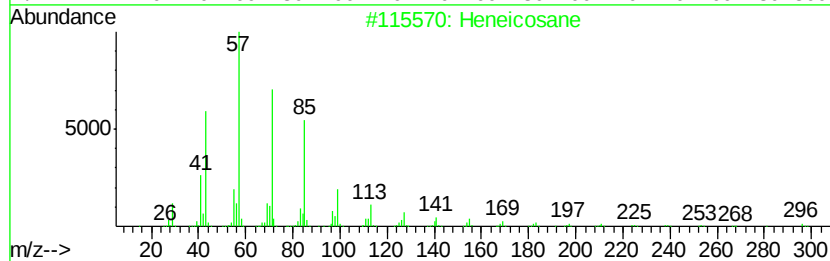
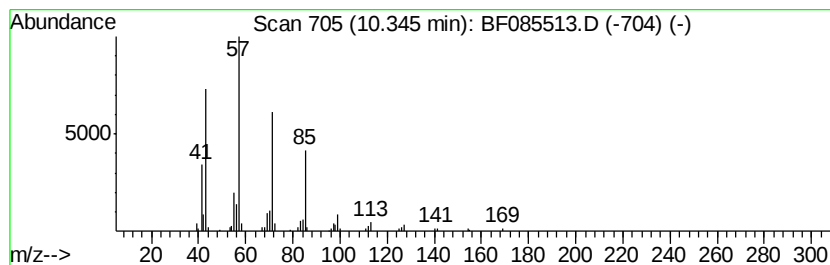
Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	2.47 ng	146078	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296	C21H44	000629-94-7 83
2	Pentadecane	212	C15H32	000629-62-9 83
3	Heptadecane	240	C17H36	000629-78-7 83
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3 83
5	Hexadecane	226	C16H34	000544-76-3 80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

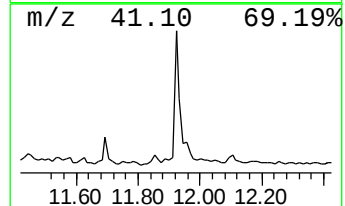
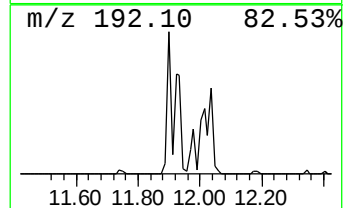
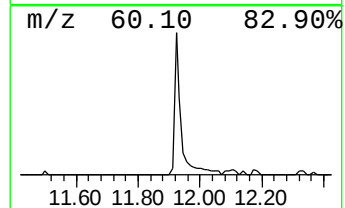
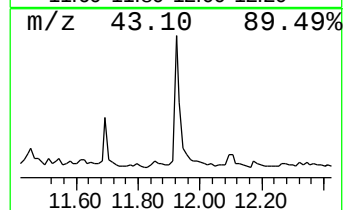
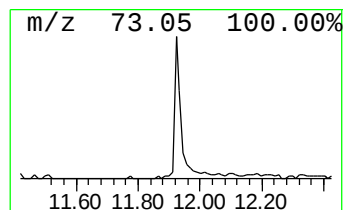
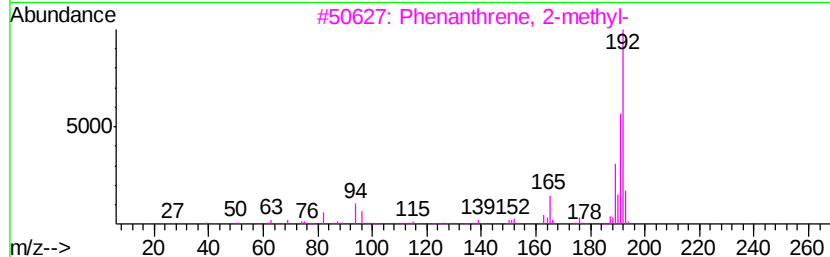
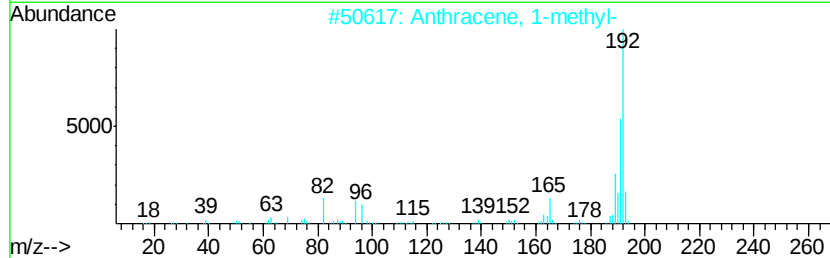
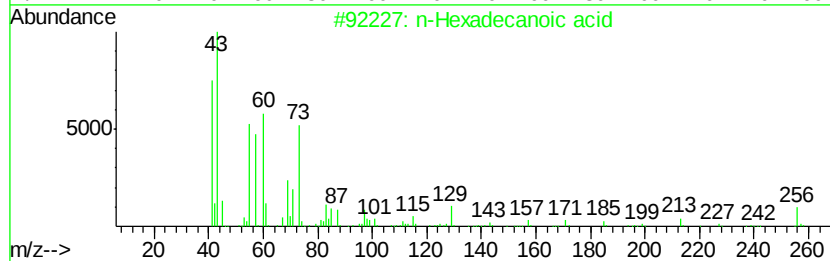
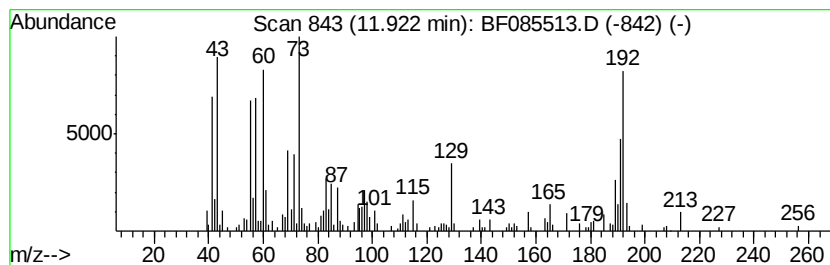
Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	3.84 ng	309316	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

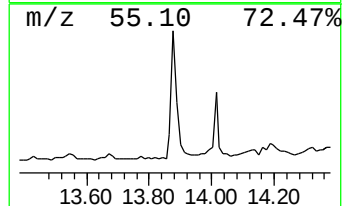
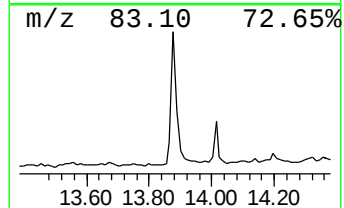
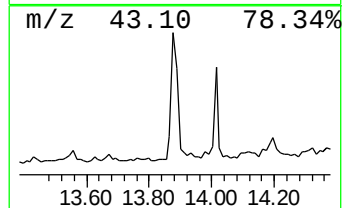
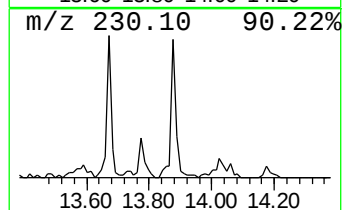
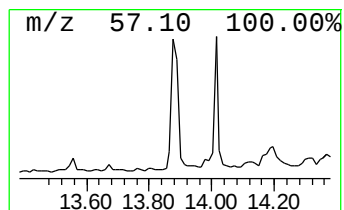
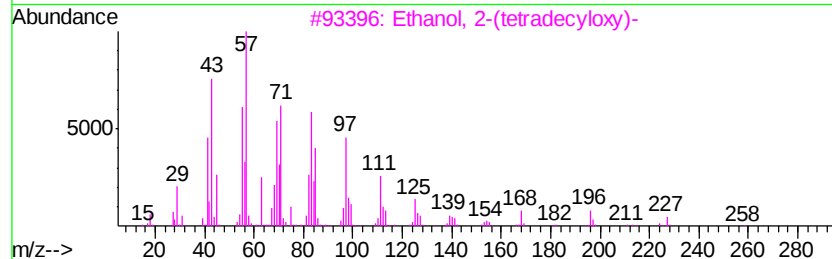
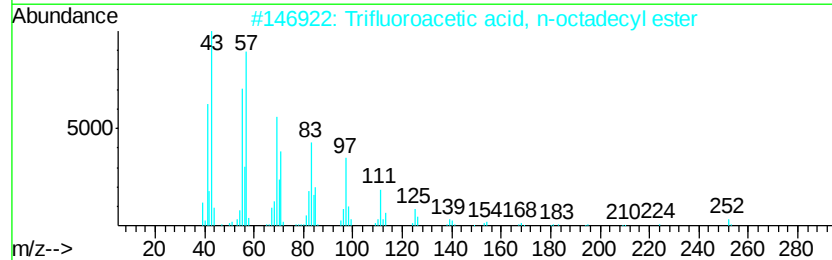
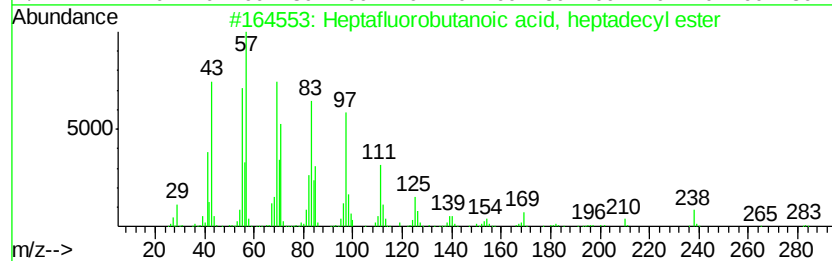
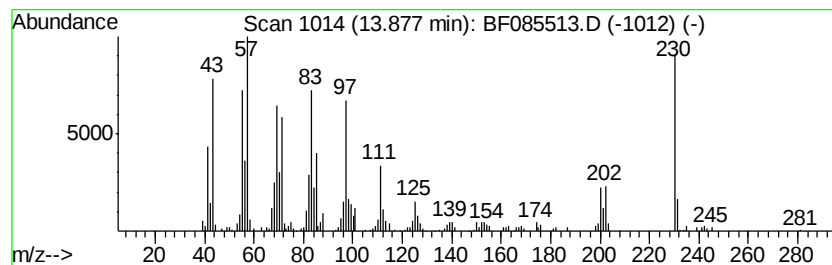
Instrument :
BNA_F
ClientSampled :
SB-15-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptafluorobutanoic acid, h... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.88	4.76 ng	341930	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	70
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	60
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	60
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	60
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	55



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

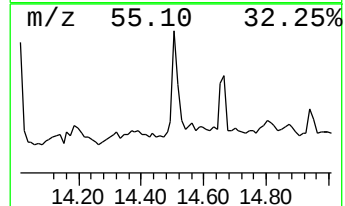
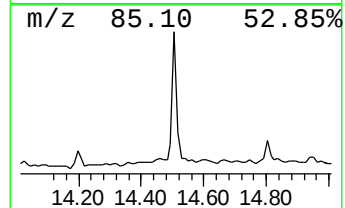
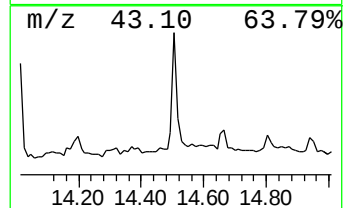
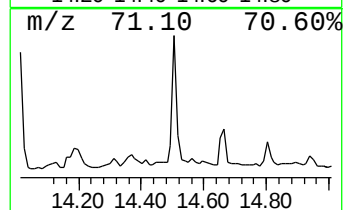
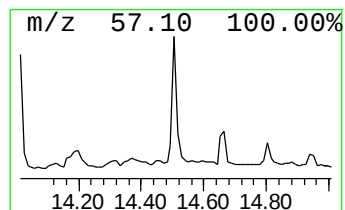
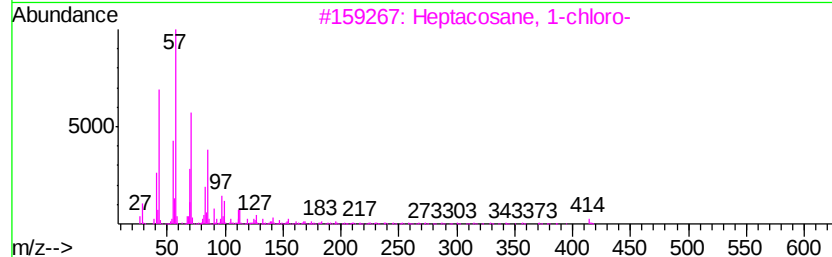
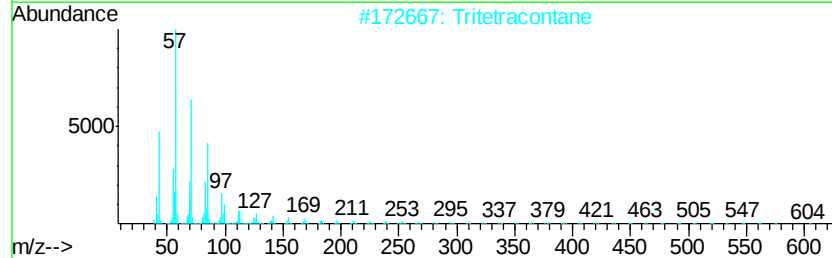
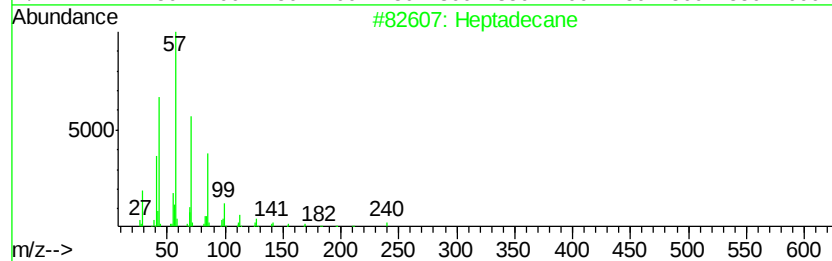
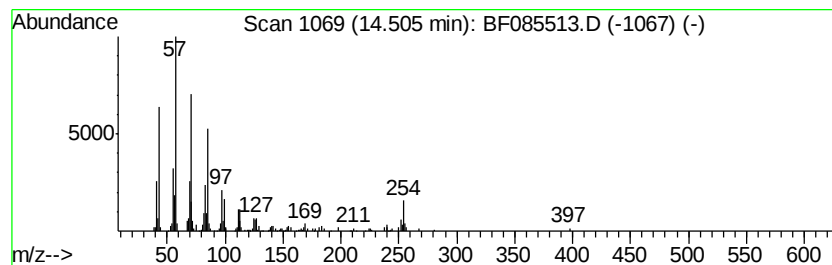
Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.31 ng	166106	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	96
2	Tritetracontane	605 C43H88	007098-21-7	83
3	Heptacosane, 1-chloro-	414 C27H55Cl	062016-79-9	83
4	Tetratetracontane	619 C44H90	007098-22-8	81
5	10-Methylnonadecane	282 C20H42	056862-62-5	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

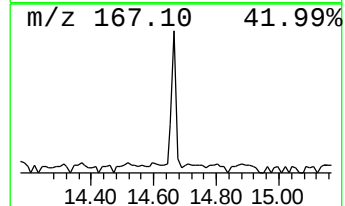
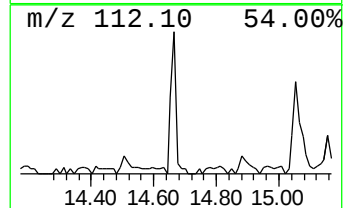
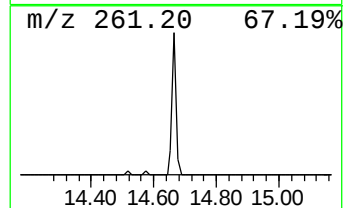
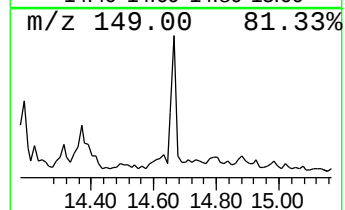
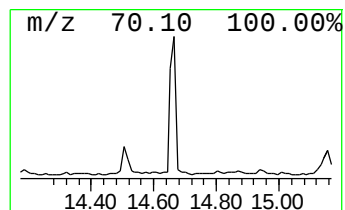
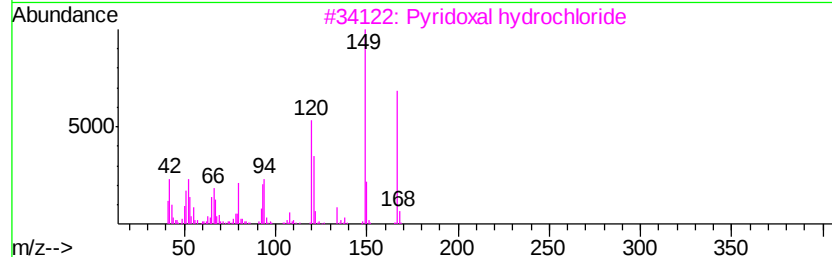
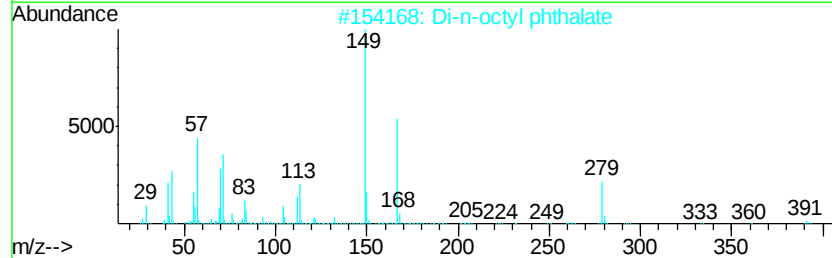
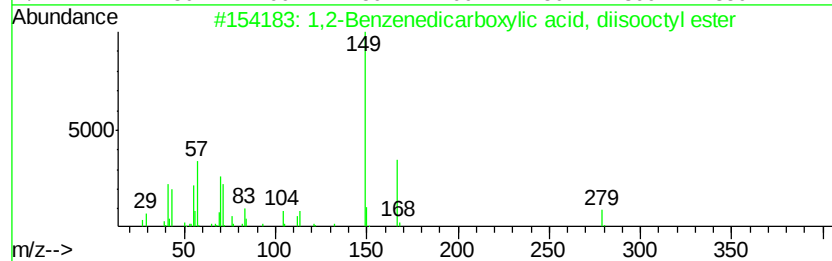
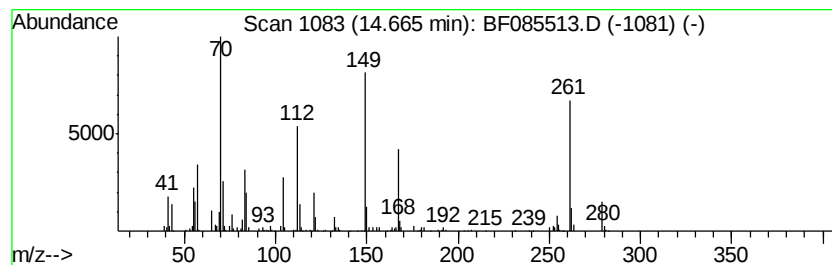
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown14.67 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.06 ng	147972	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	38
2		Di-n-octyl phthalate	390	C24H38O4	000117-84-0	38
3		Pyridoxal hydrochloride	167	C8H9NO3	000065-22-5	22
4		1,2-Benzenedicarboxylic acid, di...	330	C20H26O4	000084-61-7	22
5		Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

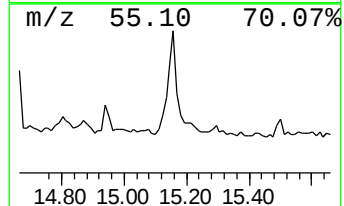
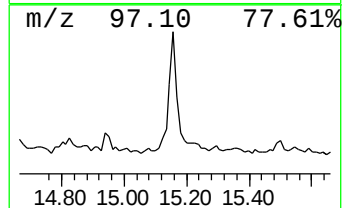
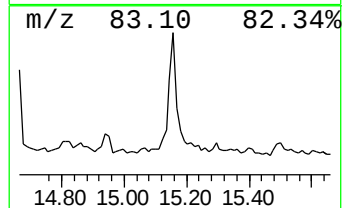
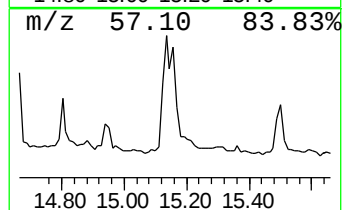
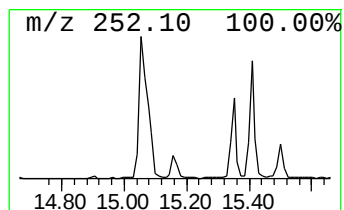
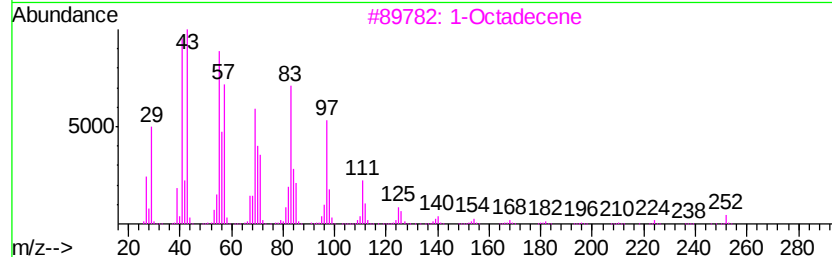
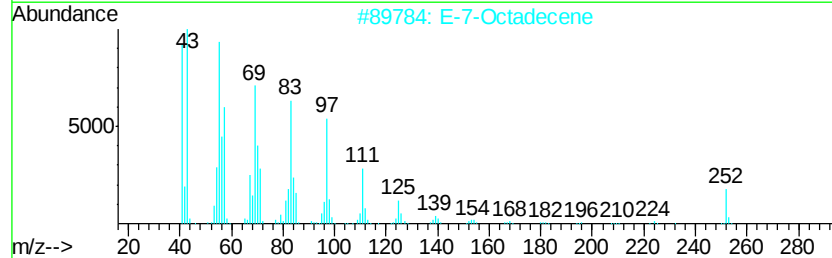
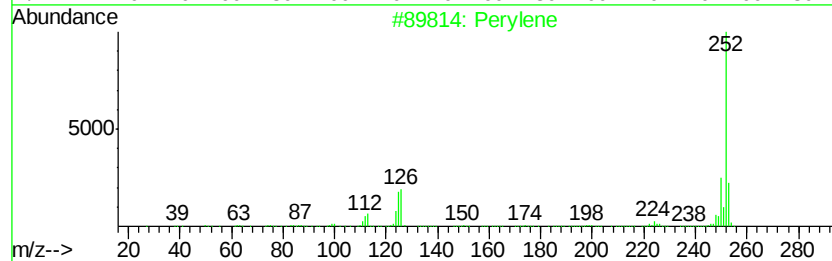
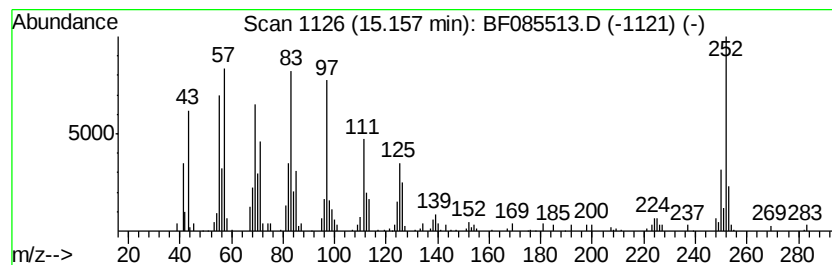
Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 E-7-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.16	4.78 ng	232694	Perylene-d12	15.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	89
2	E-7-Octadecene	252	C18H36	1000130-92-0	86
3	1-Octadecene	252	C18H36	000112-88-9	81
4	1-Octadecanol	270	C18H38O	000112-92-5	68
5	1-Docosene	308	C22H44	001599-67-3	55



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

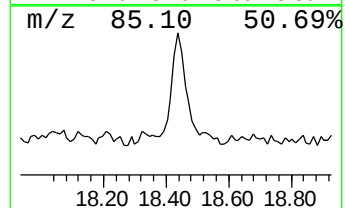
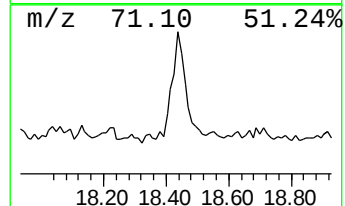
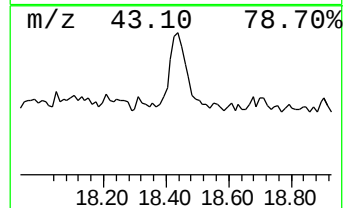
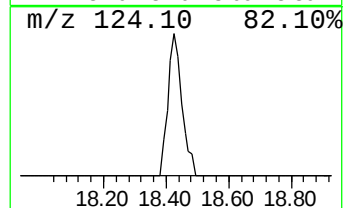
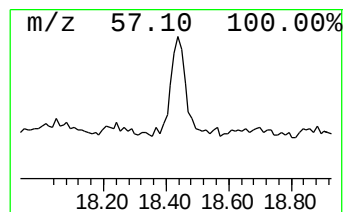
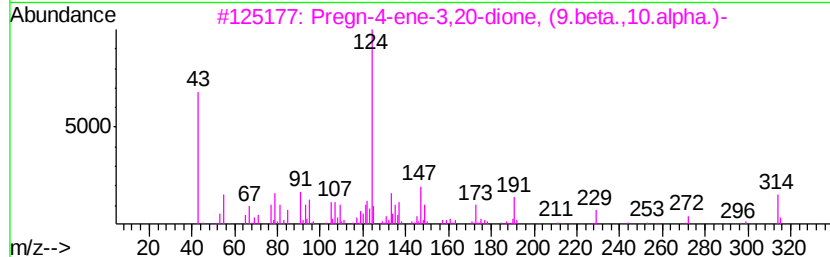
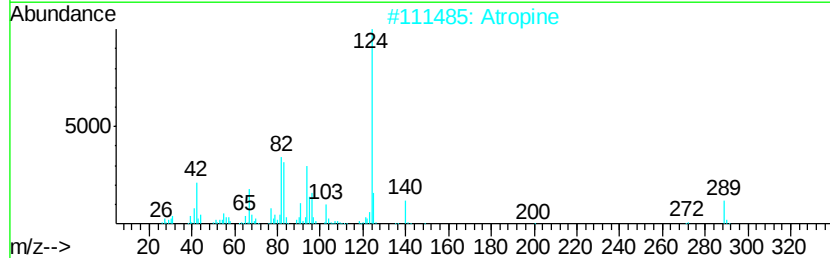
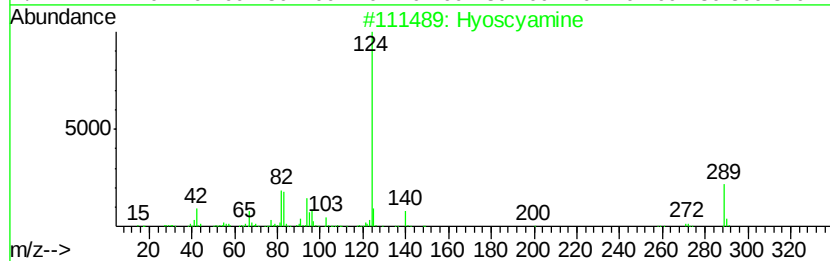
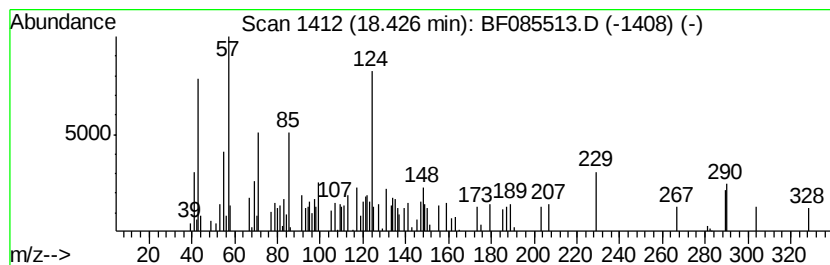
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown18.43 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	2.38 ng	116175	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hyoscyamine	289	C17H23NO3	000101-31-5	30
2		Atropine	289	C17H23NO3	000051-55-8	27
3		Pregn-4-ene-3,20-dione, (9.beta....	314	C21H30O2	002755-10-4	22
4		5-Ethylcyclopent-1-enecarboxalde...	124	C8H12O	036431-60-4	18
5		Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	002847-30-5	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085513.D
Acq On : 18 Mar 2016 1:33
Operator : UM/SJ
Sample : H1774-10
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	2.8	ng	120147	1	6.88	862596	20.0
unknown6.65	6.65	102.4	ng	4414650	1	6.88	862596	20.0
Heneicosane	10.34	2.5	ng	146078	3	9.92	1184480	20.0
n-Hexadecanoic acid	11.92	3.8	ng	309316	4	11.40	1612570	20.0
Heptafluorobutano...	13.88	4.8	ng	341930	5	14.04	1435400	20.0
Heptadecane	14.51	2.3	ng	166106	5	14.04	1435400	20.0
unknown14.67	14.67	2.1	ng	147972	5	14.04	1435400	20.0
E-7-Octadecene	15.16	4.8	ng	232694	6	15.48	974350	20.0
unknown18.43	18.43	2.4	ng	116175	6	15.48	974350	20.0